Optimization of cavitating flows simulation with data driven approach: from data assimilation to machine learning

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Abstract

This paper investigates the application of data-driven approach to the optimization of cavitating flow simulations. An evaluation of the performance of commonly used RANS models (k-e, k-w and k-w SST) is presented by comparison with high fidelity data (DNS solution and X-ray experimental measurements). An ensemble based variational method is introduced and used to reconstruct the inlet velocity and calibrate the empirical parameters in the turbulence model and the cavitation model. Machine learning approach is discussed to construct a discrepancy function of the Reynolds stresses to address the RANS model-form uncertainty.

Keywords: RANS models; cavitating flows; data assimilation; machine learning

1. Introduction

Turbulent cavitating flows occur in many engineering practical applications such as pumps, propellers and nuclear reactors. The collapse of the cavitation bubbles in these devices can produce major detrimental effects, such as flow rate fluctuations, noise, vibrations, and erosion. It is thus essential to accurately predict the behavior of unsteady cavitation, to reduce their consequences for the machinery.

After decades of efforts, the most commonly used approach to simulate these turbulent cavitating flows is still the Reynolds Averaged Navier Stokes (RANS) method combined with homogeneous cavitation models, thanks to its computational tractability. However, it is a consensus that RANS models perform poorly in cases of complex flows with separations, mean pressure gradients and/or curvatures. This limitation also leads to the poor prediction of the interactions between cavitation and turbulence in the specific case of cavitating flows. To address this issue, diverse data-driven approaches [1][2][3] have been developed in the turbulence community to improve the predictive accuracy of the RANS method from the perspective of quantifying and reducing the uncertainty due to boundary condition inconformity or model inadequacy. Especially, data assimilation methods and machine learning are both promising approaches and have demonstrated successfully their merits in the improvement of RANS model predictions. Accordingly, the goal of the present work is to investigate the application of the data-driven approaches (data assimilation and physics-informed machine learning approach) to the simulation of turbulent cavitating flows, thus contributing to an enhanced understanding of the complex flow physics.

2. Limitations of the current RANS models

2.1 CFD solver

A 2D unsteady compressible solver is applied to conduct the numerical simulation. The code is based on the coupling of a homogenous one-fluid cavitation model with a two-equation RANS turbulence model. The governing Navier-Stokes equations and transport equation of void fraction can be expressed as:

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$$\frac{\partial \omega}{\partial t} + div(F_c - F_v) = S \tag{1}$$

$$\omega = \begin{pmatrix} \rho_m \\ \rho_m u \\ \rho_m v \\ \alpha \end{pmatrix} \qquad F_c = \begin{pmatrix} \rho_m u & \rho_m v \\ \rho_m u^2 + p & \rho_m uv \\ \rho_m uv & \rho_m v^2 + p \\ \alpha u & \alpha v \end{pmatrix} \qquad F_v = \begin{pmatrix} 0 & 0 \\ \tau_{xx} & \tau_{xy} \\ \tau_{xy} & \tau_{yy} \\ 0 & 0 \end{pmatrix}$$

where $\rho_m = \alpha\rho_v + (1-\alpha)\rho_l$ is the mixture density, α is void fraction, F_c and F_v denote the convective and viscous flux densities, and S is the source term.

2.2. Comparison of RANS model prediction with high fidelity data

To eliminate the effects of the cavitation model, the comparison is performed here with non-cavitating flows. The performance of three RANS models (k-e, k-w & k-w SST) is investigated in two different canonical flows, namely i) the non-cavitating turbulent flow in a 2D Venturi type section, ii) the turbulent flow in the configuration of the Wallturb Bump [5]

A. non-cavitating flow in the Venturi type section

In the venturi-type section, the prediction on tangential velocity u with current RANS models is compared with experimental measurements based on X-ray imaging. The comparison is focused on the area immediately downstream the venturi throat along the bottom wall. The experiment set-up is detailed in [4].

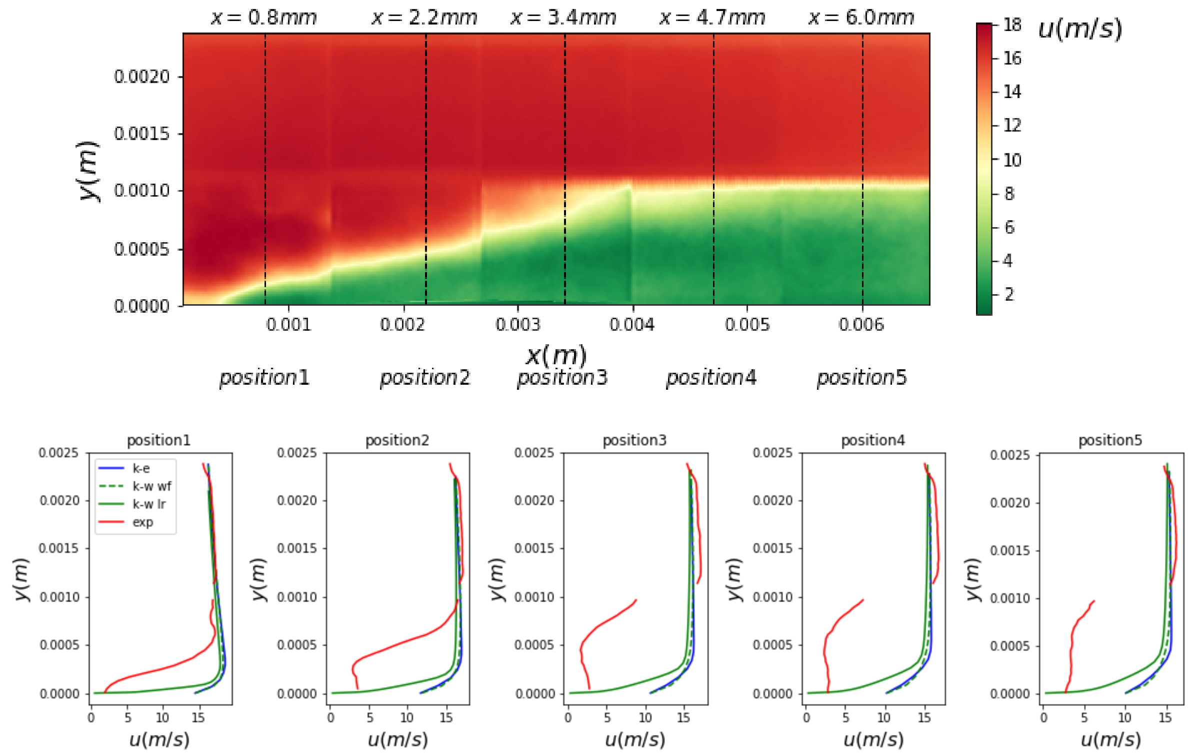

Figure 1: Top: experimental observation of velocity u; Bottom: comparison of velocity u at different positions where 'k-w wf' indicate k-w model associated with wall function and 'k-w lr' indicate k-w model associated with low Reynolds method.

From Figure 1, it can be seen that in the region far from the wall, the results of all these RANS simulations can fit well with experimental data; however, a quite large discrepancy can be figured out in the region near the wall, which indicates that the adverse pressure gradient(APG) is poorly predicted. Generally, these RANS models cannot predict the velocity u near the wall with confidence.

B. turbulence flow in configuration of Wallturb bump

The Wallturb bump geometry used in this work is presented in Figure 2. The reference DNS data [5] is used to estimate the predictive accuracy of Quantities of interest (QoIs) at wall with the RANS simulations (k-w with low Reynolds correction and k-w SST).

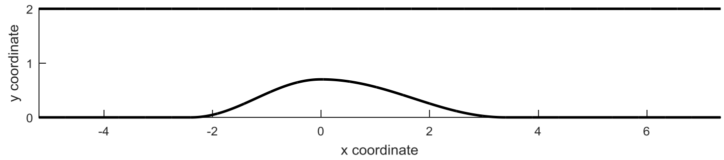

Figure 2 Profile of the Wallturb Bump

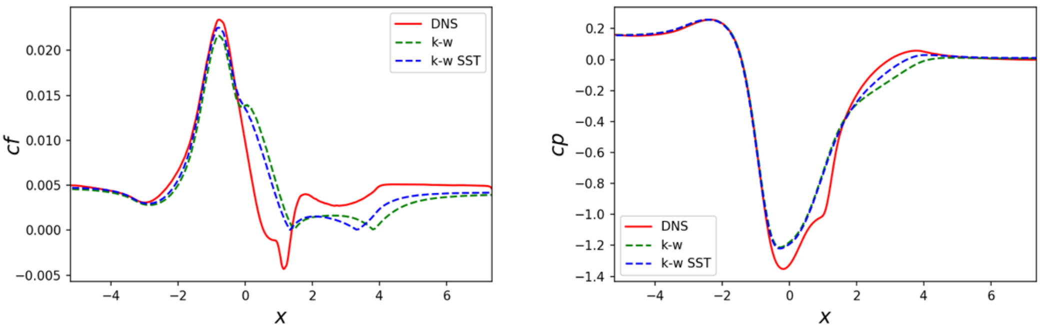

Figure 3. Comparison results of friction coefficient *cf* and pressure coefficient *cp* at the bottom wall

The friction and pressure coefficient evolutions at the bottom wall are presented in Figure 3. In the favorable pressure gradient region, it has a good agreement with DNS result with both k-w SST and k-w model; However, in the APG region, the discrepancies tend to increase for both the friction coefficient and the pressure coefficient, although the k-w SST model performs quite better than the k-w. It indicates that current RANS models perform poorly regarding the prediction in the APG region.

3. Data assimilation

In light of these limitations of the current RANS models, a data assimilation technique is conducted to improve the predictions. It has been previously demonstrated [6] that quantifying the parameter uncertainty related to the cavitation & turbulence models and the inlet conditions is feasible with the data assimilation technique. In this work, we apply an Ensemble-based variational data assimilation scheme (4DEnVar) [1] to unsteady cavitating flows. 4DEnVar is a non-intrusive method combining the variational method and an Ensemble Kalman Filter. Specifically, the formulation of the variation method uses a Monte Carlo ensemble instead of adjoint operators to estimate the prior statistics. The control vector can be expressed as:

$$\gamma = (q_0, (\alpha_n)_{n=0}^{N-1})$$

where q_0, in each cell, refers to the initial state vector formed with the components of w in equation (1), and α_n refers to the inlet boundary condition and/or the model parameters at time n. After making a first guess about the optimal vector to initiate the background (prior knowledge) $\gamma^{(e)}$, stochastic modeling can be performed to sample N_{en} ensemble of realizations around the background. Then the control vector γ (posterior knowledge) is expressed as:

$$\gamma = \gamma^{(e)} + E'\beta \qquad E' = (\gamma^{(1)} - \gamma^{(e)}, \gamma^{(2)} - \gamma^{(e)}, \dots, \gamma^{(N_{en})} - \gamma^{(e)}) \tag{2}$$

As for the observation (reference data), the stochastic model extension can be expressed as

$$y_n = \mathrm{h}(q_n) + \epsilon_n \tag{3}$$

Where h is the observation operator that maps the state space to the observation space, and ϵ_n is the possible measurement error, which is assumed to be a zero-mean, uncorrelated Gaussian random field.

Based on the Bayesian inference, maximizing a posterior (MAP) estimation amounts to minimizing a cost function (4). This cost function is composed of two parts: (i) the difference between the control vector and the background and (ii) the difference between the CFD results based on the prior knowledge and the observation, weighed by the inverse of background covariance B and observation covariance C, respectively.

$$J = \frac{1}{2}\left\|\gamma - \gamma^{(e)}\right\|_{B^{-1}}^{2} + \sum_{n=0}^{N}\frac{1}{2}\parallel d_n - y_n \parallel_{C^{-1}}^{2} \tag{4}$$

Where $d_n = \mathrm{h}(\gamma^{(e)}) + H_n^{'}\beta,\quad H_n^{'} = \left(\mathrm{h}\left(q_n^{(1)}\right) - \mathrm{h}\left(q_n^{(e)}\right), \dots, \mathrm{h}\left(q_n^{(N_{en})}\right) - \mathrm{h}\left(q_n^{(e)}\right)\right)$

with $\|*\|_{\mathrm{B}^{-1}}^{2} = *^{\mathrm{T}}\,\mathrm{B}^{-1}\,*;\ \|*\|_{\mathrm{C}^{-1}}^{2} = *^{\mathrm{T}}\,\mathrm{C}^{-1}\,*; B \simeq \frac{1}{N_{en}-1}E'E'^{T}\ ;\ C \simeq \epsilon\epsilon^{T}$

$$\frac{\partial J}{\partial \beta} = (N_{en} - 1)\beta + {H_n'}^{\mathrm{T}}C^{-1}(d_n - y_n), \qquad \frac{\partial^2 J}{\partial \beta^2} = (N_{en} - 1)\mathrm{I} + {H_n'}^{\mathrm{T}}C^{-1}H_n' \tag{5}$$

In order to minimize the cost function (4), one iteration of Newton CG method is performed with (5). The obtained β is used to update the optimal vector γ according to (2). This iterative process is continued until the maximum iteration number is reached.

4. Machine learning approach

The data assimilation approach can infer improved boundary conditions and empirical parameters for the turbulence and cavitation models. However, it can only provide the uncertainty within the framework of the RANS approach, while the main source of uncertainty in RANS simulations is due to the constitutive assumptions of the RANS modeling. Therefore, over the past few years, machine learning approaches have been developed to address these model-form uncertainties.

The physics informed machine learning approach (PIML) [2] has been applied to construct the discrepancy function in terms of Reynolds stress. In cavitating flows, by taking the X-ray experimental data as training data set, it is expected to extend the application of the PIML framework from steady flow at low Reynolds numbers to unsteady flow at high Reynolds numbers, and further to cavitating flows. It is of primary importance to define the input features in cavitating condition. Besides the ten features suggested in [2], some other features like the homogeneous density, the void fraction and void fraction gradient should also be embedded. Moreover, the challenge of propagation from Reynolds stress to the QoIs (mean velocity and pressure) needs to be tackled.

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